

CONTENTS OF VOLUME 77

NUMBER 1—SEPTEMBER 1992

A shape model for molecular ordering in nematics By A. FERRARINI, G. J. MORO, P. L. NORDIO and G. R. LUCKHURST	1
The r_s structure of oxetane as studied by NMR spectroscopy in a nematic medium By A. L. ESTEBAN and M. P. GALACHE	17
Percolation of three-dimensional square-well fluid mixtures By D. M. HEYES	29
The crystal structure of CBrF_3 by high-resolution powder neutron diffraction By A. JOUANNEAUX, A. N. FITCH and J. K. COCKCROFT	45
An MCSCF/MP2 study of methylene insertion-abstraction reactions with C-H and C-Cl bonds By F. BERNARDI, A. BOTTONI and M. A. ROBB	51
Hydrogen bonded complexes of HCl with CO, C_2H_2, C_2H_4, PH_3, H_2S, HCN, H_2O and NH_3. Correlated quantum chemical calculations of geometries, energetics, vibrational frequencies and ^{35}Cl quadrupole coupling constants By G. B. BACSKAY	61
Reaction yield detected magnetic resonance and magnetic field effect studies of radical pairs containing electronically excited organic radicals By S. N. BATCHELOR, K. A. McLAUCHLAN and I. A. SHKROB	75
Calculated rovibrational energy levels and infrared spectrum of $\text{He-C}_2\text{H}_2$ By T. SLEE, R. J. LE ROY and C. E. CHUAQUI	111
Dipole moment, electric field gradient and hyperfine coupling constants of the $X^2\Pi$ state of PS: <i>ab initio</i> MRD-CI studies By S. P. KARNA and F. GREIN	135
Local polarizability calculations with localized orbitals in the uncoupled Hartree-Fock approximation By P.-O. ÅSTRAND and G. KARLSTRÖM	143
Molecular dynamics simulation of the TIPS model of 1,2-dichloroethane in the liquid phase By C. MILLOT and J. L. RIVAIL	157
Molecular motion and vibrational dephasing in a model of liquid N_2O_4 By T. KATŌ, M. OOBATAKE, K. MACHIDA and S. HAYASHI	177
Analytical treatment of the quadratic and nonrelativistic Renner-Teller effect for a triatomic molecule in a Π electronic state. I. High energy limit By A. AGUILAR, M. GONZÁLEZ and L. V. POLUYANOV	193

NUMBER 2—10 OCTOBER 1992

Analytical treatment of the quadratic and nonrelativistic Renner-Teller effect for a triatomic molecule in a Π electronic state. II. High energy and high angular momentum limit By A. AGUILAR, M. GONZÁLEZ and L. V. POLUYANOV	209
Collision frequencies and mean collision parameters in the Lennard-Jones system By F. DEL RÍO and A. GIL-VILLEGAS	223
Molecular dynamics simulation of polarizable water by an extended Lagrangian method By D. VAN BELLE, M. FROEYEN, G. LIPPENS and S. J. WODAK	239
The structure and molecular dynamics of solid <i>n</i>-decylammonium chloride By E. C. REYNHARDT, S. JURGA and K. JURGA	257
<i>Ab initio</i> potential-energy curves for the molecular ions NeH^+ and ArH^+ By D. M. HIRST, M. F. GUEST and A. P. RENDELL	279
Calculations of second light-scattering virial coefficients of linear and quasi-linear molecules By C. GRAHAM	291

A density functional study of nematic-smectic A-solid transitions of parallel hard spherocylinders By HONG XU	311
Exchange-Coulomb potential energy curves for He-He, and related physical properties By R. A. AZIZ, M. J. SLAMAN, A. KOIDE, A. R. ALLNATT and W. J. MEATH	321
Molecular dynamics investigations of the electrostatic interactions in liquid carbonyl sulphide By H. STASSEN, TH. DORFMÜLLER and J. SAMIOS	339
Simulation results and corresponding states correlation for pure rigid molecular fluids By G. M. SOWERS and S. I. SANDLER	351
Theoretical calculations of the nuclear magnetic shielding tensors for the ethylenic carbon atoms in cyclopropenes By C. M. SMITH, R. D. AMOS and N. C. HANDY	381
Pulsed ultraviolet laser photolysis of substituted phenyl azosulfonates. Wavelength dependent effects By D. FRANZKE, B. VOIT, O. NUYKEN and A. WOKAUN	397

NUMBER 3—20 OCTOBER 1992

Water structure in aqueous solutions of tetramethylammonium chloride By J. TURNER, A. K. SOPER and J. L. FINNEY	411
Solute-solute correlations in aqueous solutions of tetramethylammonium chloride By A. K. SOPER, J. TURNER and J. L. FINNEY	431
Towards an accurate intermolecular potential for water By C. MILLOT and A. J. STONE	439
<i>Ab initio</i> bending potential-energy curves for Rydberg states of H₂O By D. M. HIRST and M. S. CHILD	463
Monte Carlo calculation of interaction energies for van der Waals complexes By G. J. TAWA, P. WHITLOCK, K. E. SCHMIDT and J. W. MOSKOWITZ	477
On Connor's connection formula across a potential well, generalized to phase-integral approximations of arbitrary order By A. AMAHA and F. KARLSSON	491
Calculated dissociation energies of the alkali metal monoxides NaO and KO: Basis set superposition error and symmetry lowering By E. P. F. LEE, T. G. WRIGHT and J. M. DYKE	501
Shear and rotational viscosity coefficients of two nematic liquid crystals By H.-H. GRAF, H. KNEPPE and F. SCHNEIDER	521
Distinctive high frequency spectrum of liquid methyl fluoride By T. GROCHULSKI and A. GERSCHEL	539
Rovibronic ²B₁(Π_g)-²A₁ spectrum of the BH₂ radical By M. BROMMER, P. ROSMUS, S. CARTER and N. C. HANDY	549
Cross-sections for charge exchange of atoms on multiply charged ions. Charge exchange of N²⁺(2p) on He(1s²) in the eV energy range By E. E. NIKITIN and A. I. REZNIKOV	563
An analysis of NMR spinning sidebands of homonuclear two-spin systems using Floquet theory By T. NAKAI and C. A. McDOWELL	569
Tubular graphitic carbon structures By YING-DUO GAO and W. C. HERNDON	585

NUMBER 4—NOVEMBER 1992

Correlated motion of two particles in a fluid. II. Molecular dynamics results By P. FLENER and F. J. VESELY	601
Solvent-solute hydrogen bonding in dilute solutions of CN⁻ and CH₃CN in water and methanol By M. FERRARIO, I. R. McDONALD and M. C. R. SYMONS	617

On the electrostatic potential in crystalline systems where the charge density is expanded in Gaussian functions By V. R. SAUNDERS, C. FREYRIA-FAVA, R. DOVESI, L. SALASCO and C. ROETTI	629
Electrochemical potentials in the grand canonical ensemble. Some formal and numerical results for confined ionic systems By P. SLOTH	667
Direct correlation between lithium cation and carboxyl anion in highly concentrated aqueous solution By K. ICHIKAWA, S. KOTANI, M. IZUMI and T. YAMANAKA	677
The dielectric constant and the site-site direct correlation function of the RISM-2 theory for polar polyatomic molecular fluids By M. OHBA and H. NOMURA	689
An algebraic approach to calculating rotation-vibration spectra of polyatomic molecules By A. B. MCCOY and E. L. SIBERT III	697
Long-range and overlap effects on collision-induced properties By P. W. FOWLER and A. J. SADLEJ	709
The hardness factor in rotational inelastic scattering By J. C. BELCHIOR, J. N. MURRELL and S. D. BOSANAC	727
Density and temperature dependence of spectral moments in depolarized light scattering by rare gases By B. M. LADANYI, A. BARREAU and B. DUMON	735
Pair correlations in an NaCl-SPC water model. Simulations versus extended RISM computations By G. HUMMER, D. M. SOUMPAIS and M. NEUMANN	769

Research Notes

Effect of rotation on molecular shape By D. SHEN and H. O. PRITCHARD	787
Origin of the linear dependence with atomic number of correlation energies in neutral atoms By N. H. MARCH and P. WIND	791
Monte Carlo simulation of the melting behaviour of $A_{12}B$ Lennard-Jones heteroclusters By M. J. GRIMSON	797

NUMBER 5—10 DECEMBER 1992

Application of cell theory to the thermodynamic properties of hard dumbbell solids By E. P. A. PARAS, C. VEGA and P. A. MONSON	803
Using monomer properties to obtain integrated intensities for vibrational transitions of van der Waals complexes By S. A. C. McDOWELL, C. R. LE SUEUR, A. D. BUCKINGHAM and A. J. STONE	823
Simulations of adsorption on microporous interfaces By J. VERMESSE and D. LEVESQUE	837
Integral equations for conventional correlation functions of simple dimerizing fluids By E. S. YAKUB	845
Thermodynamic and scaling behaviour in finite diffusion-limited aggregation By M. A. LÓPEZ-QUINTELA and M. C. BUJÁN-NÚÑEZ	857
Theoretical estimate of <i>ortho</i>-<i>para</i> separation coefficients for H_2 and D_2 on A-type zeolites for small and medium coverage By A. V. LARIN and V. S. PARBUZIN	869
Concentration effects on absolute depolarized Rayleigh ratios and effective polarizability derivatives of CS_2 in liquid mixtures with CCl_4 By F. STREHLE and TH. DORFMÜLLER	893
Combination of computer simulation methods and optimized cluster theory in determining equilibrium properties of electrolyte solutions. I. General expressions and application to pure water By A. D. TROKHYMCHUK, M. F. HOLOVKO, E. SPOHR and K. HEINZINGER	903
The LiC_2H_2 and NaC_2H_2 adducts. Is sodium-vinylidene observed in matrix reaction of sodium with acetylene? By MINH THO NGUYEN, TAE-KYU HA and M. YOSHIMINE	921

Intraband vibronic coupling between excited electronic states in <i>cis</i>-polyacetylene by Raman resonance scattering	
By P. SASSI and R. S. CATALIOTTI	937
A comment on recent proposals for the calculation of vibration-rotation energies in more-than-three atom molecules	
By X. CHAPUISAT, A. BELAFHAL, A. NAUTS and C. IUNG	947
Rotational motion of Brownian particles with surface charge	
By N. V. BRILLIANTOV and N. G. VOSTRIKOVA	957
Hard body models for chiral nematic liquid crystals	
By G. T. EVANS	969
Perturbation theory of the quadrupolar Kihara fluid	
By T. BOUBLÍK	983
Far infrared spectra of (HF)₂ and (HF)₃ in solid argon	
By L. ANDREWS, S. R. DAVIS and R. D. HUNT	993

Research Notes

The dipolar hard sphere fluid. Hypernetted chain approximation revisited	
By E. LOMBA, C. MARTÍN and M. LOMBARDERO	1005
On the simple derivation of approximate integral equations for triplet and higher-order distribution functions of homogeneous fluids	
By O. A. PIZIO	1011
Erratum	1019

NUMBER 6—20 DECEMBER 1992

Effect of a density-dependent potential on the phase behaviour of fluids	
By B. SMIT, T. HAUSCHILD and J. M. PRAUSNITZ	1021
Phase equilibria for associating Lennard-Jones fluids from theory and simulation	
By J. K. JOHNSON and K. E. GUBBINS	1033
The dielectric dispersion surface for the nitrogen molecule in the gas phase	
By R. S. BARBIERI and R. A. BONHAM	1055
On the VDWI mixing rules applied to conformational binary mixtures at infinite dilution. A systematic improvement	
By D. A. JONAH and U. K. DEITERS	1071
Accurate dipole polarizability for Cl₂(X¹Σ_g⁺)	
By G. MAROULIS	1085
Exponentially damped Breit-Pauli Hamiltonian for the description of positronium decay and other high energy processes	
By R. J. BUENKER	1095
The orientations and dynamics of ethanol guest molecules in the clathrate of Dianin's compound. A ²H-nuclear magnetic resonance single crystal study	
By T. BERNHARD, H. ZIMMERMANN and U. HAEBERLEN	1123
The selfdiffusion coefficient and viscosity of the hard sphere fluid revisited: a comparison with experimental data for xenon, methane, ethene and trichloromethane	
By K. R. HARRIS	1153
A theoretical study of the molecules BeF and BeF⁺ in their lowest-lying electronic states	
By F. R. ORNELLAS, F. B. C. MACHADO and O. ROBERTO-NETO	1169
The vibrational spectrum of FBrCO. An experimental and theoretical study	
By Y. ZHAO and J. S. FRANCISCO	1187
Variational calculation of the ro-vibrational states of Na₂⁺	
By F. WANG and E. I. VON NAGY-FELSOBUKI	1197
The Gaussian thermostat, phase space compression and the conjugate pairing rule	
By D. J. EVANS and A. BARANYAI	1209
Intra and intermolecular structure in the condensed phases of ethylene, ethane and carbon dioxide by neutron diffraction	
By A. K. ADYA and C. J. WORMALD	1217
Index of authors (with the titles of papers)	1247

